Overview of Resonance Region Covariance Data Generation Efforts for Sensitivity/Uncertainty Analyses

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OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Outline

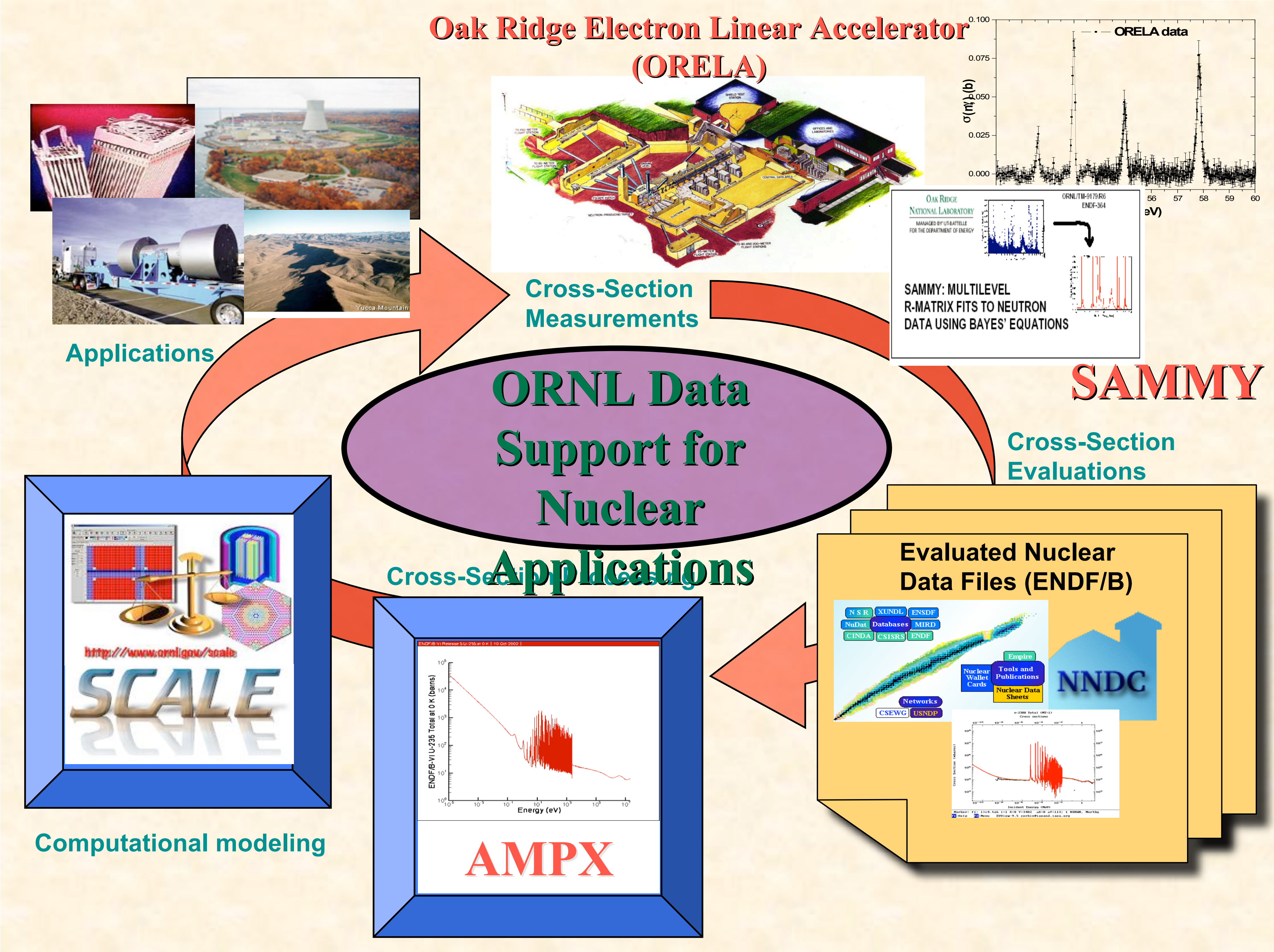
- ORNL Nuclear Systems Analysis & Design Safety
- Current Status of ENDF/B Covariance Data
- ORNL Covariance Data Generation Efforts
- What to Expect with ENDF/B-VII
- ORNL Covariance Data Processing Improvements
- Sensitivity/Uncertain Methods for Propagating Cross-Section Uncertainty Data to Application of Interest
- Summary

ORNL Nuclear Systems Analysis & Design

- ORNL provides technical support to DOE/NNSA (NA-11) **N**uclear **C**riticality **S**afety **P**rogram (NCSP)—develop and maintain state-of-the-art radiation transport and nuclear data capabilities for criticality safety applications

- Software and data developments under DOE/NCSP
  - AROBCAD—**A**pplicable **R**anges of **B**ounding **C**urves and **D**ata
    - Sensitivity/uncertainty (S/U) analysis tools (1-D and 3-D) can be used to provide fissile system sensitivity information and propagate cross-section uncertainty data to calculated quantities of interest
    - TSUNAMI software released with SCALE 5.0 in June 2004
  - ORNL Nuclear Data program integrated with radiation transport methods capabilities:
    - ORELA cross-section measurements for resonance region
    - Nuclear modeling methods development (SAMMY)
    - Cross-section evaluation and preparation of ENDF/B nuclear data files
    - Cross-section processing methods development for generating nuclear data libraries (AMPX)
  - NCSP addressing "high-priority" data needs for criticality safety applications in DOE complex—including covariance data

- Data and Methods work should be of direct benefit to the AFCI/GEN-IV Program


Oak Ridge Electron Linear Accelerator (ORELA)
ORELA data
Cross-Section Measurements
Applications
Yucca Mountain
SAMMY: MULTILEVEL R-MATRIX FITS TO NEUTRON DATA USING BAYES' EQUATIONS
SAMMY
ORNL Data Support for Nuclear Applications
Cross-Section Evaluations
Evaluated Nuclear Data Files (ENDF/B)
NSR
XUNDL
ENSDF
NuDat
Databases
MIRD
CINDA
CSISRS
ENDF
Empire
Nuclear Wallet Cards
Tools and Publications
Nuclear Data Sheets
Networks
CSEWG
USNDP
NNDC
Cross-Section Processing
Energy (eV)
AMPX
http://www.ornl.gov/scale
SCALE
Computational modeling

Current Status of ENDF/B Covariance Data

- **Cross-section covariance data needed for S/U capabilities in SCALE**
- **ENDF/B-VI has limited amount of covariance data**
  - 49 out of 344 evaluations have covariance information
    - Contrast with 27 evaluations in ENDF/B-V with covariance data
    - Many important nuclides do not have covariance data in ENDF/B-VI
  - Resonance parameter covariance data only available for ^{241}Am, ^{23}Na, ^{240}Pu, ^{242}Pu
  - Resonance parameter covariances limited to SLBW or MLBW—does not account for interference effects between resonances
- **Shortage of covariance data is problem for International Data Projects as well**
  - JEFF
  - JENDL
  - BROND
  - CENDL

Covariance Data in ENDF/B-VI

	Th-232	*	Sc-45
	Pu-242		Cr-50,52,53,54
	Au-197		Fe-54,56,57,58
*	Bi-209		Ni-58,60,61,62,64
	Pu-240		Mn-55
	Am-241	*	Cu-63,65
*	V		F-19
	Co-59	*	Re-185,187
*	Y-89		Pb-206,207,208
*	Ti-46,47,48		Si
	Na-23	*	Nb
	U-238	*	In
	Al-27		U-235
	Pu-241		

* New in ENDF/B-VI

Covariance Data in ENDF/B-V

N-14	Ni
H-1	Li-7
O-16	Au-197
Li-6	Pb
B-10	Np-237
C	Pu-242
F-19	Am-241
Na-23	Pu-240
Al-27	Pu-241
Si	Th-232
Mn	U-235
Fe	Pu-239
Co-59	U-238
Cr	

_ Missing from ENDF/B-VI

ORNL Covariance Data Generation Efforts

- **Re-evaluating all ENDF/B materials to obtain covariance data is a multi-year task**
- **Need covariance data much sooner**
- **ORNL has "three-pronged" approach for addressing covariance data needs**
  - Traditional cross-section evaluation approach
  - Retroactive covariance data generation for resonance region—methodology developed by Nancy Larson (ORNL)
  - Approximate covariance generation—methodology developed by Mark Williams (ORNL)

ORNL Covariance Data Generation Efforts

- **Traditional Evaluation Approach—Most rigorous but time consuming**

- **SAMMY R-matrix software analysis approach**
  - Resonance analysis based on measured cross-section data
  - Uses Bayes' method (generalized least squares) to find parameter values.
  - Uses R-matrix theory, Reich-Moore approximation (default) or multi- or single-level Breit-Wigner theory.
  - Generates covariance and sensitivity parameters for resonance region (generalized least squares).

- **Covariance matrix generated during the resonance analysis as part of the ENDF/B evaluation preparation**

- **Historical note:**
  - Demand was only for the resonance parameters needed to produce cross-section data
  - ENDF/B formats prior to ENDF/B-VII not adequate to transmit resonance parameter covariances—more robust resonance formats in ENDF/B-VII
  - Result—evaluator did not keep covariance matrices and only the cross-section data have been preserved in evaluations

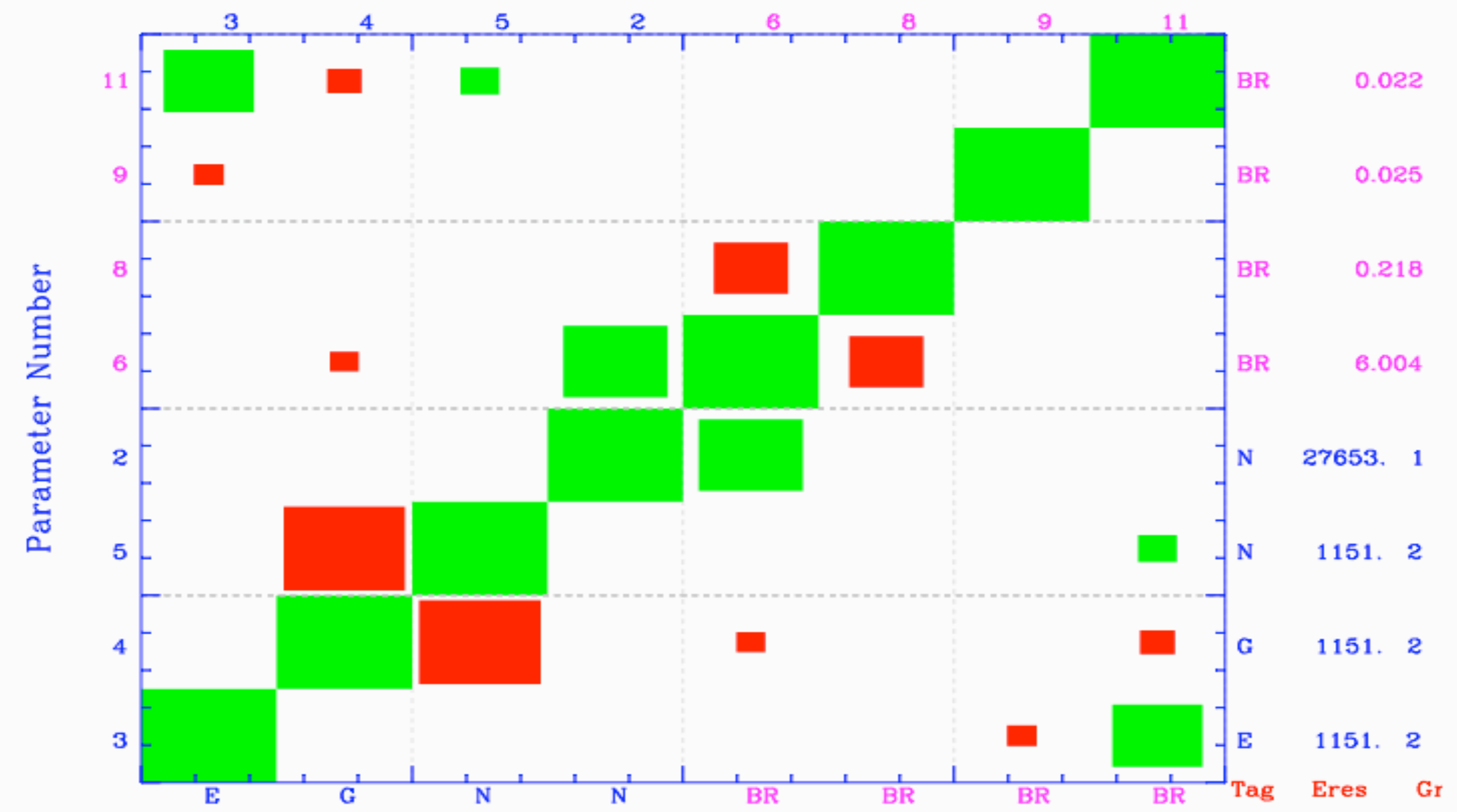
- **New ORNL evaluation efforts focus on providing cross-section data with covariance data**
  - ^{35}Cl, ^{37}Cl, ^{39}K, ^{41}K, ^{55}Mn, ^{19}F
  - ^{103}Rh, ^{133}Cs, ^{143}Nd, ^{149}Sm, ^{151}Sm

ORNL Covariance Data Generation Efforts

- **Recently developed GUI software to manipulate and visualize SAMMY resonance parameter covariance data to support evaluation efforts—RADCOP**
- **Typical resonance evaluation → 100s or 1000s of parameters**
  - **Evaluator needs to examine and display subsets of parameter covariance matrix**
- **RADCOP capabilities:**
  - 1-D and 2-D plots of parameter correlations for specified energy ranges
  - Plot formats facilitate rapid identification of important off-diagonal correlations
  - Output of ENDF/B resonance parameters and corresponding covariance parameters for Reich-Moore formalism
  - Visualization for new ENDF/B-VII resonance formats in development

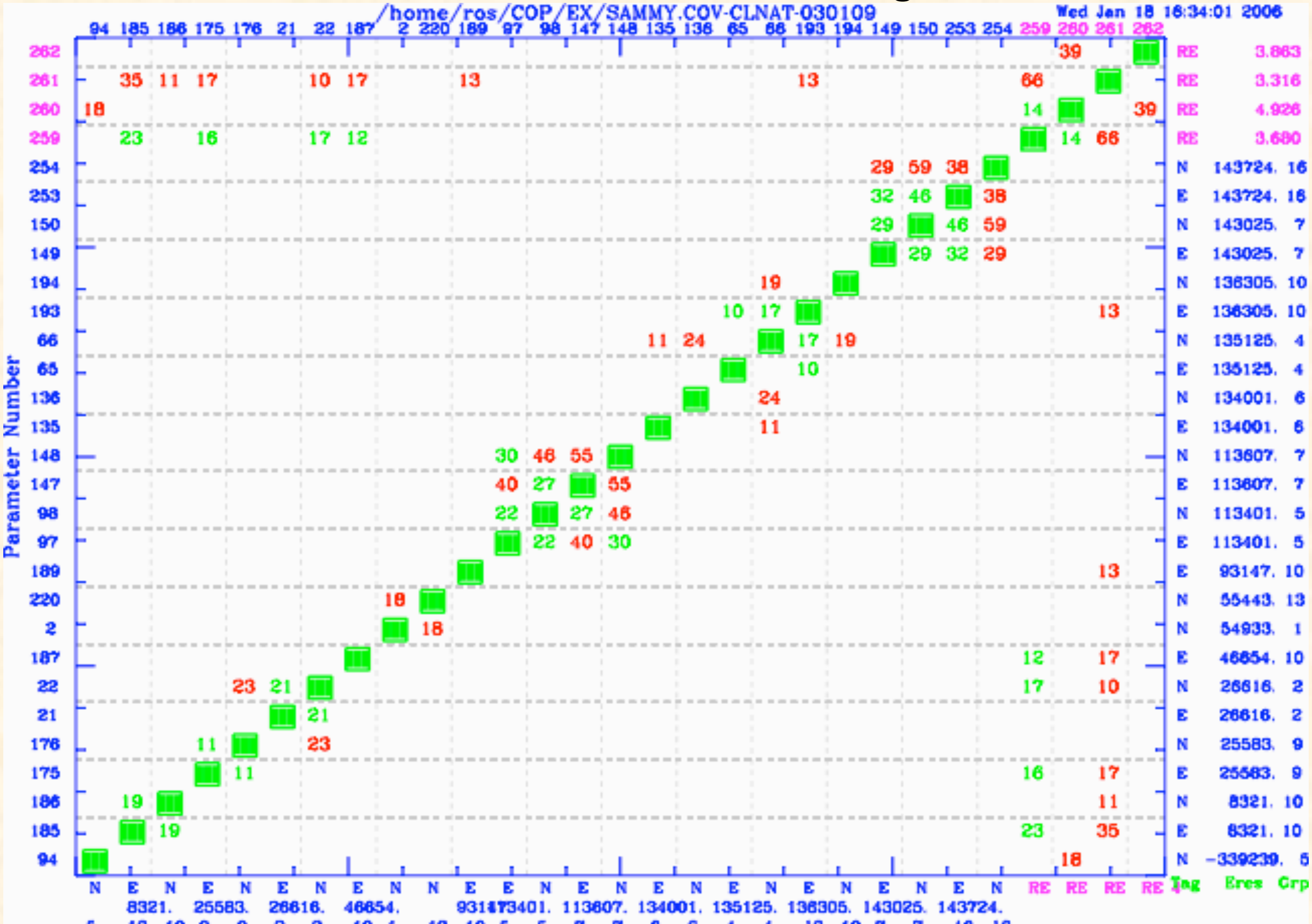
ORNL Covariance Data Generation Efforts

RADCOP 2D Correlation Plot: ^{37}Cl Positive (negative) correlations are shown in green (red). The label BR denotes broadening parameters.



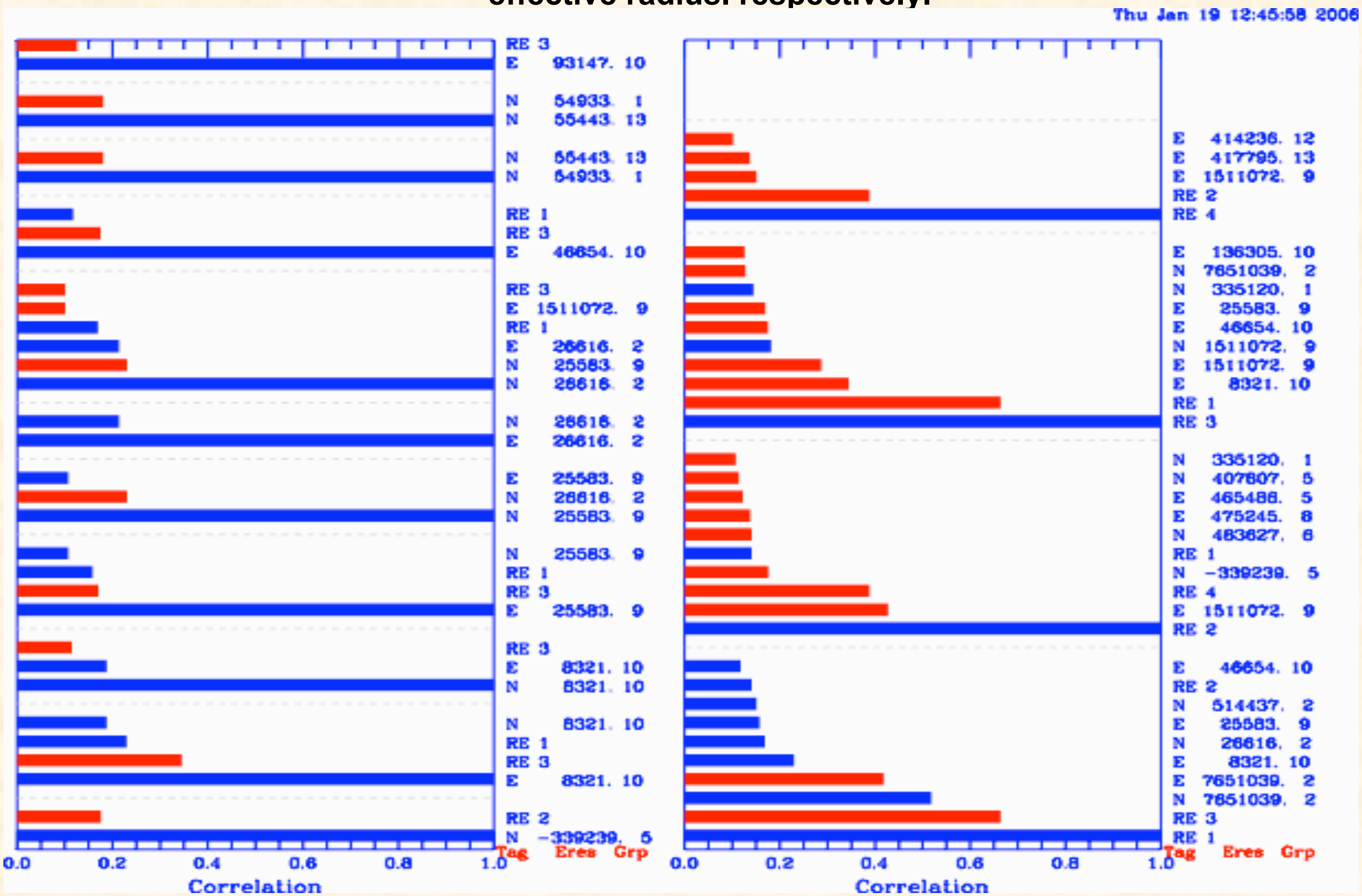
ORNL Covariance Data Generation Efforts

RADCOP 2D Plot: ^{37}Cl with numerical off-diagonal correlations



ORNL Covariance Data Generation Efforts

RADCOP 1D Plot: ^{37}Cl showing extreme off-diagonal correlations. Blue (red) bars indicate positive (negative) correlations. Tags E, N, and RE, denote resonance energy, neutron width, and effective radius, respectively.

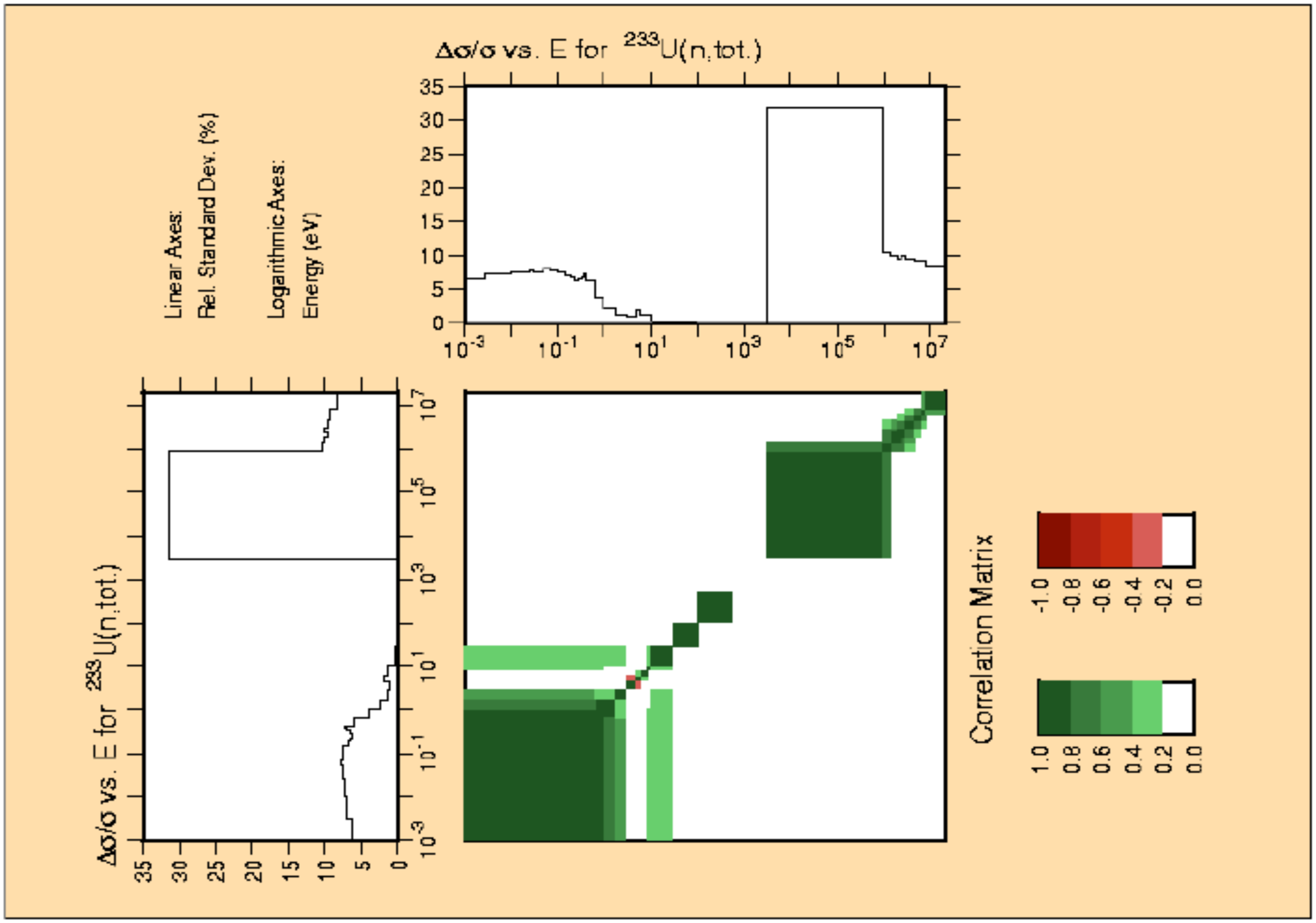


ORNL Covariance Data Generation Efforts

- **Retroactive Evaluation Approach—less rigorous relative to traditional evaluation approach but faster**
- **Resonance evaluation already exists—keep existing ENDF/B resonance parameters but add resonance parameter covariance data**
- **Larson (ORNL) has implemented capability in SAMMY software to retroactive generate resonance parameter covariance data**
  1. Pick representative experimental data sets covering the energy range of existing evaluation
  2. Do simultaneous fit to all those data sets
     - Use existing ENDF/B res. parameters as initial values
     - Flag all resonance parameters—treated as variables in the fitting procedure
  3. Check whether output parameter values are very different from input—should be fairly consistent
  4. Assume that the output parameter covariance matrix is a reasonable approximation to use in conjunction with the original (input) parameter values
  5. Export output parameter covariance matrix into ENDF/B resonance-parameter format
- **FY2005: Luiz Leal (ORNL) used approach to retroactively generate covariance data for ^{233}U and Gd isotopes—will be available in ENDF/B-VII**

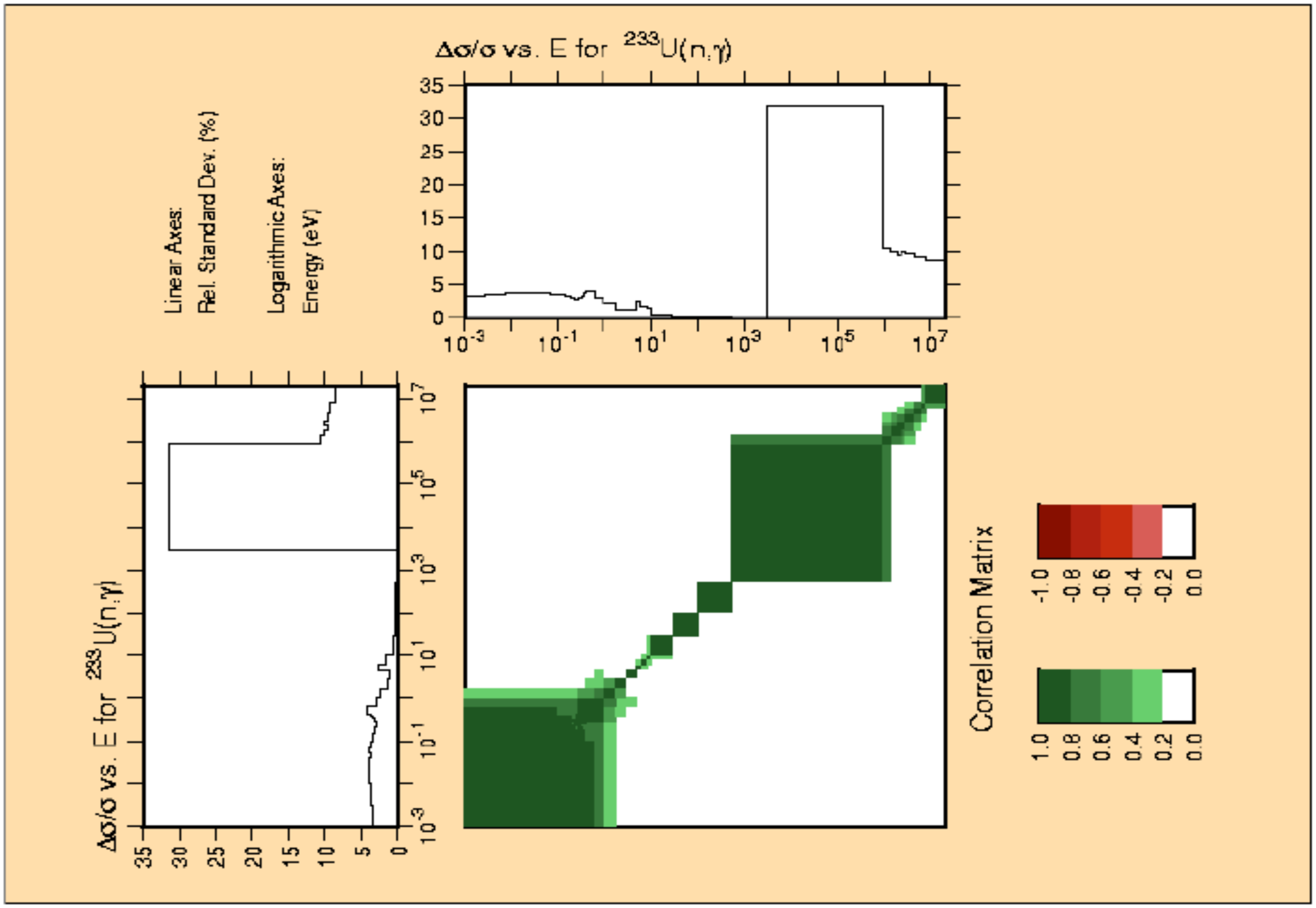
ORNL Covariance Data Generation Efforts

ERRORJ Processed Covariance (^{233}U Total)



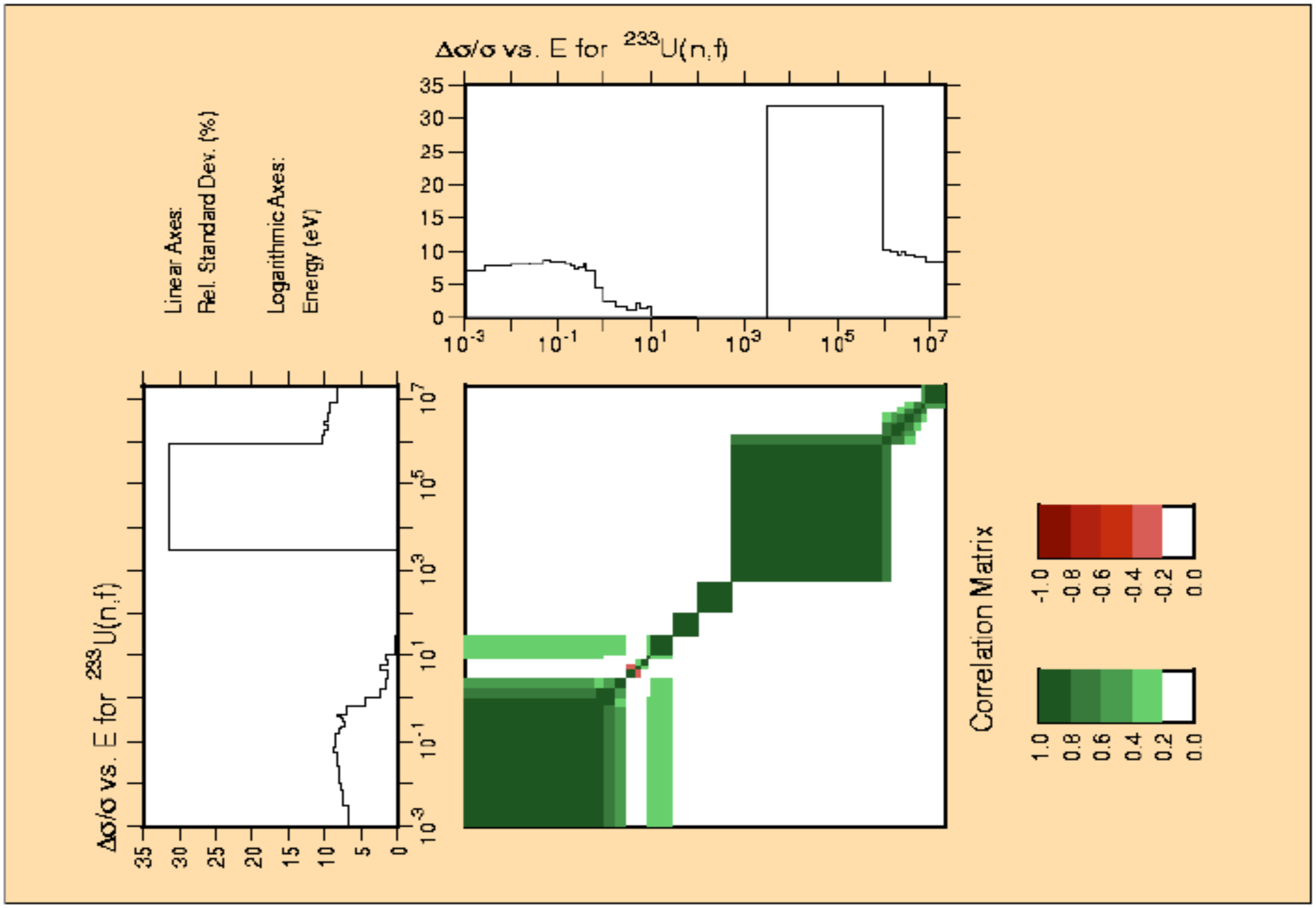
ORNL Covariance Data Generation Efforts

ERRORJ Processed Covariance (^{233}U Capture)



ORNL Covariance Data Generation Efforts

ERRORJ Processed Covariance (^{233}U Fission)



ORNL Covariance Data Generation Efforts

- **Approximate Approach—least rigorous but fast**
  - Only used for nuclides that do not have covariance data
  - Will not be distributed with ENDF/B evaluations—only used to fill covariance data gaps in SCALE covariance library

- **Approximate cross-section covariances for energy ranges:**
  - Thermal (< 0.5 eV)
  - Epithermal (resonance region)
  - Fission-source region

- **Thermal range**
  - Capture or fission:

$$\mathrm{Cov}(\sigma_g, \sigma_{g'}) \approx \sigma_g \, \sigma_{g'} \frac{\mathrm{Var}(\sigma_0)}{\sigma_0^2}; \quad \sigma_0 = 2200 \text{ m/sec value}$$

  - Elastic:

$$\mathrm{Cov}(\sigma_g, \sigma_{g'}) \approx \sigma_g \, \sigma_{g'} \frac{\mathrm{Var}(\sigma_p)}{\sigma_p^2}; \quad \sigma_p = \text{potential}$$

ORNL Covariance Data Generation Efforts

- **Approximate Approach (cont'd)**

- **Epithermal range**
  - Capture:

$$\mathrm{Cov}(\sigma_g, \sigma_{g'}) \approx \sigma_g \, \sigma_{g'} \frac{\mathrm{Var}(I_c)}{I_c^2}; \quad I_c = \text{capture resonance integral}$$

  - Fission:

$$\mathrm{Cov}(\sigma_g, \sigma_{g'}) \approx \sigma_g \, \sigma_{g'} \frac{\mathrm{Var}(I_f)}{I_f^2}; \quad I_f = \text{fission resonance integral}$$

  - Elastic:

$$\mathrm{Cov}(\sigma_g, \sigma_{g'}) \approx \sigma_g \, \sigma_{g'} \frac{\mathrm{Var}(\sigma_p)}{\sigma_p^2}; \quad \sigma_p = \text{potential scatter}$$

- **Fission-source range**

$$\mathrm{Cov}(\sigma_g, \sigma_{g'}) \approx \sigma_g \, \sigma_{g'} \frac{\mathrm{Var}(\sigma_\chi)}{\sigma_\chi^2}; \quad \sigma_\chi = \int \sigma(E)\,\chi(E)\,dE; \quad \sigma_\chi = \text{fission-equivalent xsec}$$

ORNL Covariance Data Generation Efforts

- **Approximate Approach (cont'd)**
- **Uncertainties in thermal data, resonance integrals, and σ_p were taken from Mughabghab's data compilation**

example thermal data (σ_0)

Nuclide	σ_c (barns) ENDF/B-VI	σ_c (barns) Mughabghab	% uncertainty Mughabghab
H-1	3.320E-01	3.326E-01	0.2
Xe-135	2.636E+06	2.650E+06	4.1
Sm-149	4.017E+04	4.014E+04	1.5
Np-137	1.810E+02	1.759E+02	1.6

ORNL Covariance Data Generation Efforts

- **Prepare "comprehensive" library for release with SCALE 5.1 in FY 2006**
- **Covariance data needed for SCALE sensitivity/uncertainty tools—TSUNAMI**
- **AMPX (PUFF module) used to process available ENDF/B covariance data and generate multigroup covariance data**
- **Supplement covariance library with approximate covariances σ_c, σ_f, σ_s, $\overline{\nu}$ using:**
  - thermal cross-section (σ_0) uncertainty for E < 0.5 eV with full correlation
  - resonance integral (I_f or I_c) uncertainty for 0.5 eV < E < 5 keV with full correlation
  - potential cross-section uncertainty up to 5 keV with full correlation
- **Covariance libraries:**
  - 44-group library for criticality safety and reactor physics applications
  - 47-group library for shielding applications
  - 56 nuclides have ENDF/B covariances
  - ~270 nuclides have approximate covariances

What to Expect with ENDF/B-VII

- **Changes with ENDF/B-VII (Summer 2006)**
  - Larson (ORNL) developed new resonance parameter format (LRF=7) that permits representation of all particle channels
  - Larson also developed new "Compact Covariance Format" (CCF) to transmit resonance parameter covariance data for resonance evaluations having "large" number of resonances (e.g., ^{233}U, ^{235}U ^{238}U, etc.)
  - Existing Reich-Moore (RM) resonance parameter covariance format will be used to transmit resonance covariance data for majority of nuclides
  - New covariance evaluations expected with initial ENDF/B-VII release:
    - ^{152,153,154,155,156,157,158,160}Gd, ^{233}U, and ^{232}Th
    - ORNL expects to have ^{235}U and ^{238}U resonance parameter covariance data by March 2006
- **Processing code status for preparing cross-section libraries with new covariance data files**
  - **NJOY: ERRORR updates needed to process RM, LRF=7, and CCF data**
  - **ERRORJ: Process RM format but cannot process LRF=7 and CCF**
  - **AMPX: PUFF-IV recently developed to process all covariance formats**

Covariance Data Processing Improvements

- **PUFF-IV module development for AMPX**
  - Complete rewrite of PUFF-III code in F90.
  - Object oriented design as far as possible in F90.
  - Results are the same as in PUFF-III within rounding errors
  - Automatic test cases comparing PUFF-III results and PUFF-IV results
- **Resonance-parameter Covariance processing**
  - Derivatives are calculated from File 2 using SAMRML
  - Group averages of covariances are calculated using the above derivatives
  - Only resolved region data can be handled
  - Resolved region: lrf=1,2,3 and lcomp=0,1,2, lrf=7 and lcomp=2 (lrf=1,2 resonance parameters are translated to Reich-Moore formalism before calculating derivatives)
  - Internal test cases to ensure proper working of group averaging
  - Automatic test cases to compare results with SAMMY generated group averaged covariance data

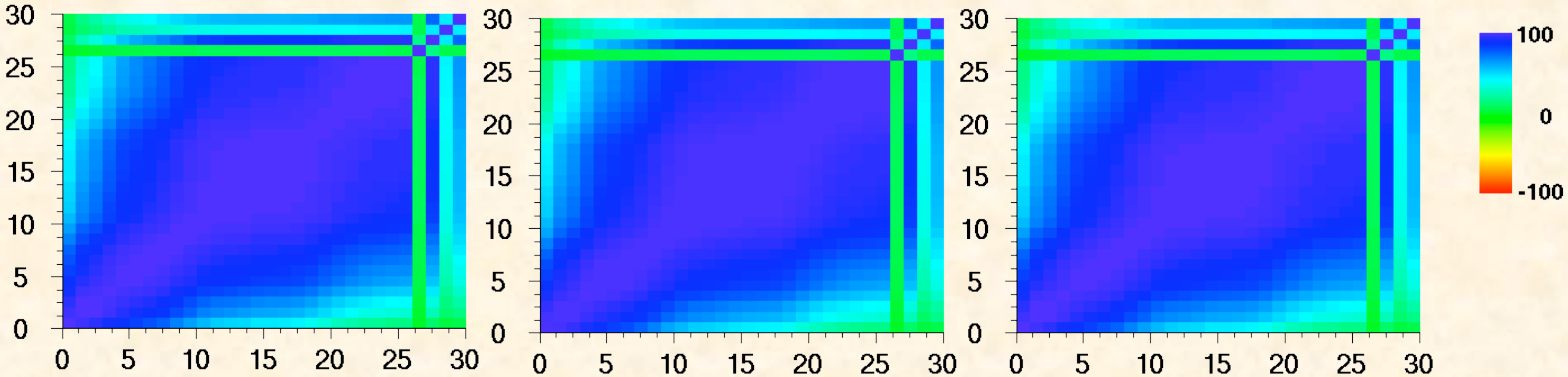
Covariance Data Processing Improvements

^{158}Gd resolved region only: Total cross section – flat flux

JENDL-3.2, for comparison with Errorj: lrf=3, lcomp =1

Correlation matrices

Sammy **Puff-IV** **Errorj**



Std. deviation

Largest absolute difference:

Errorj -Sammy: $1.21*10^{-5}$

Errorj -Puff-IV: $5.22*10^{-6}$

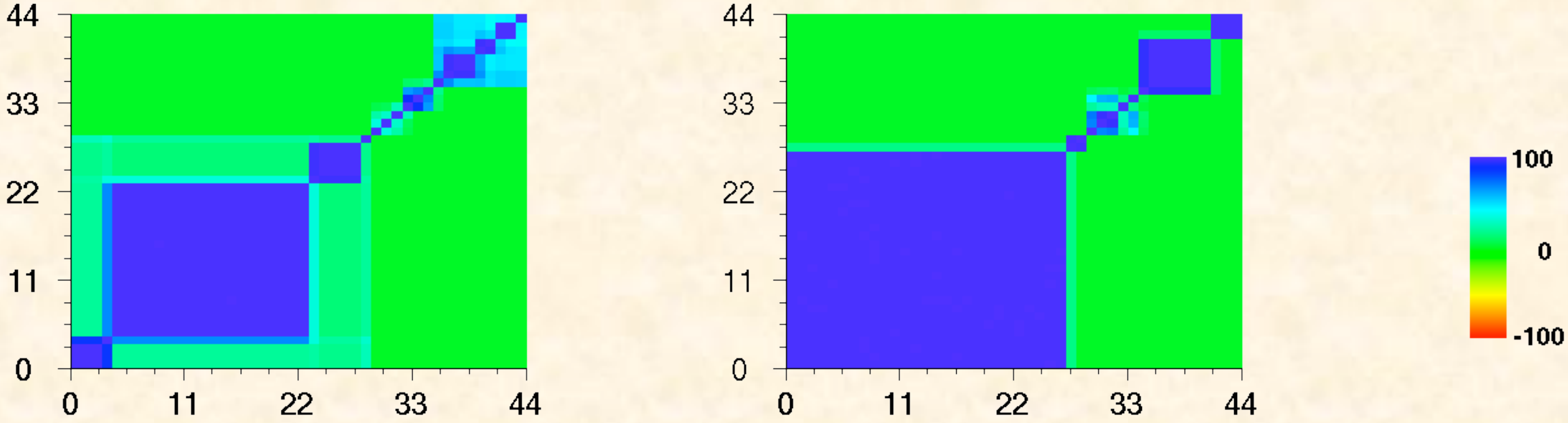
Sammy - Puff-IV: $1.30*10^{-5}$

Covariance Data Processing Improvements

^{23}Na: File 33 and File 32 processing – flat flux

ENDF/B-VI MOD2
lrf=2, lcomp=0
Sensitivity analysis for File 32
Puff-III and Puff-IV (identical results)

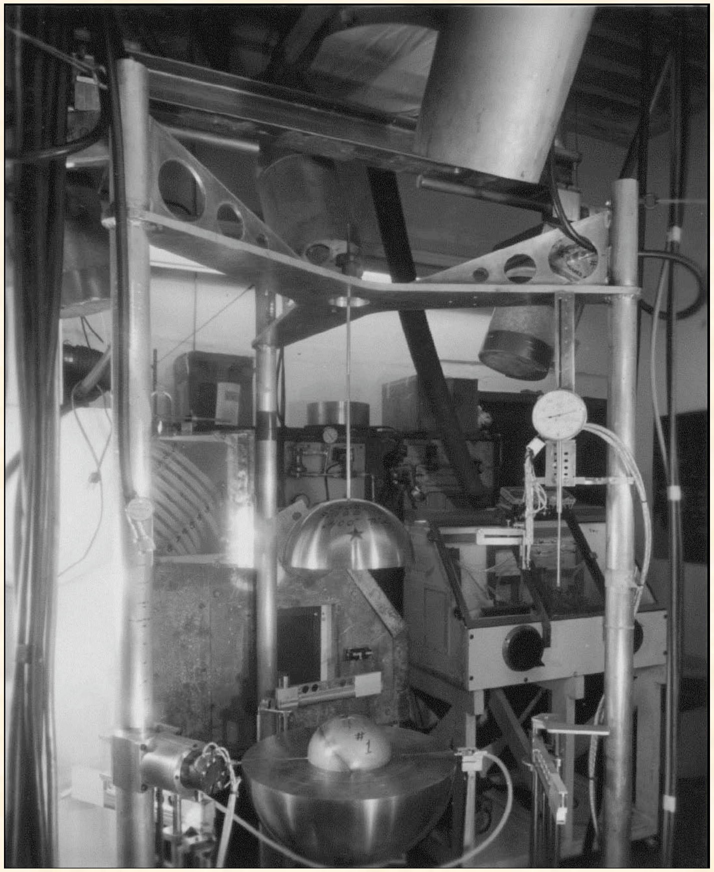
Total cross section　　　　Capture cross section



Benchmark Calculations with ENDF/B-VI 238 Group Structure (ICSBEP)

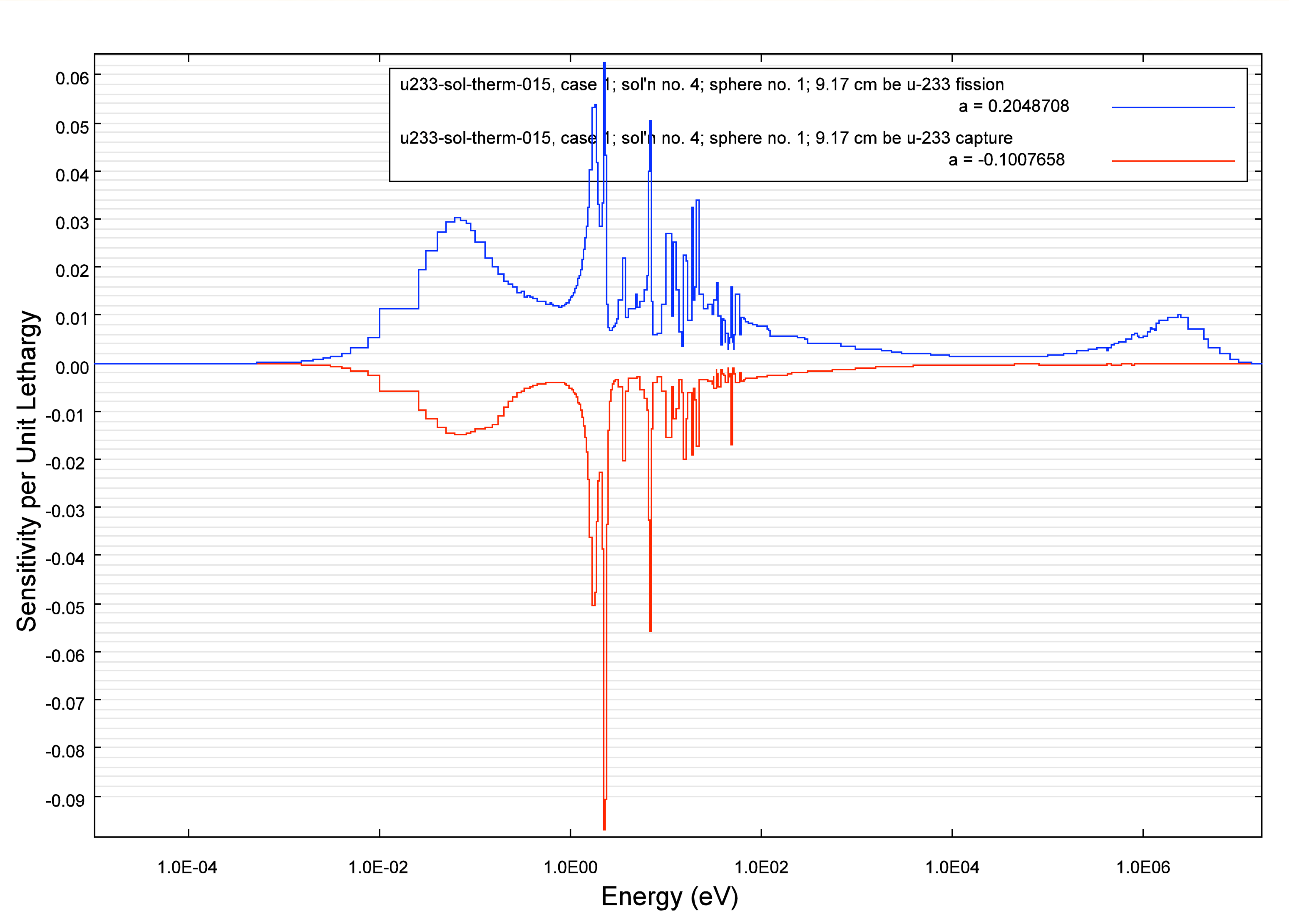
uct001 (2 cases) not used	ust003 (10 cases)
umf001 (1 case)	ust004 (8 cases)
umf002 (2 cases)	ust005 (2 cases)
umf003 (2 cases)	ust006 (25 cases)
umf004 (2 cases)	ust008 (1 case)
umf005 (2 cases)	ust009 (4 cases)
umf006 (1 case)	ust012 (8 cases)
usi001 (33 cases)	ust013 (2 cases)
ust001 (5 cases)	ust014 (16 cases)
ust002 (16 cases)	ust015 (31 cases)
Total: 175 cases	

Overview of Experiment (u233-sol-therm-015)

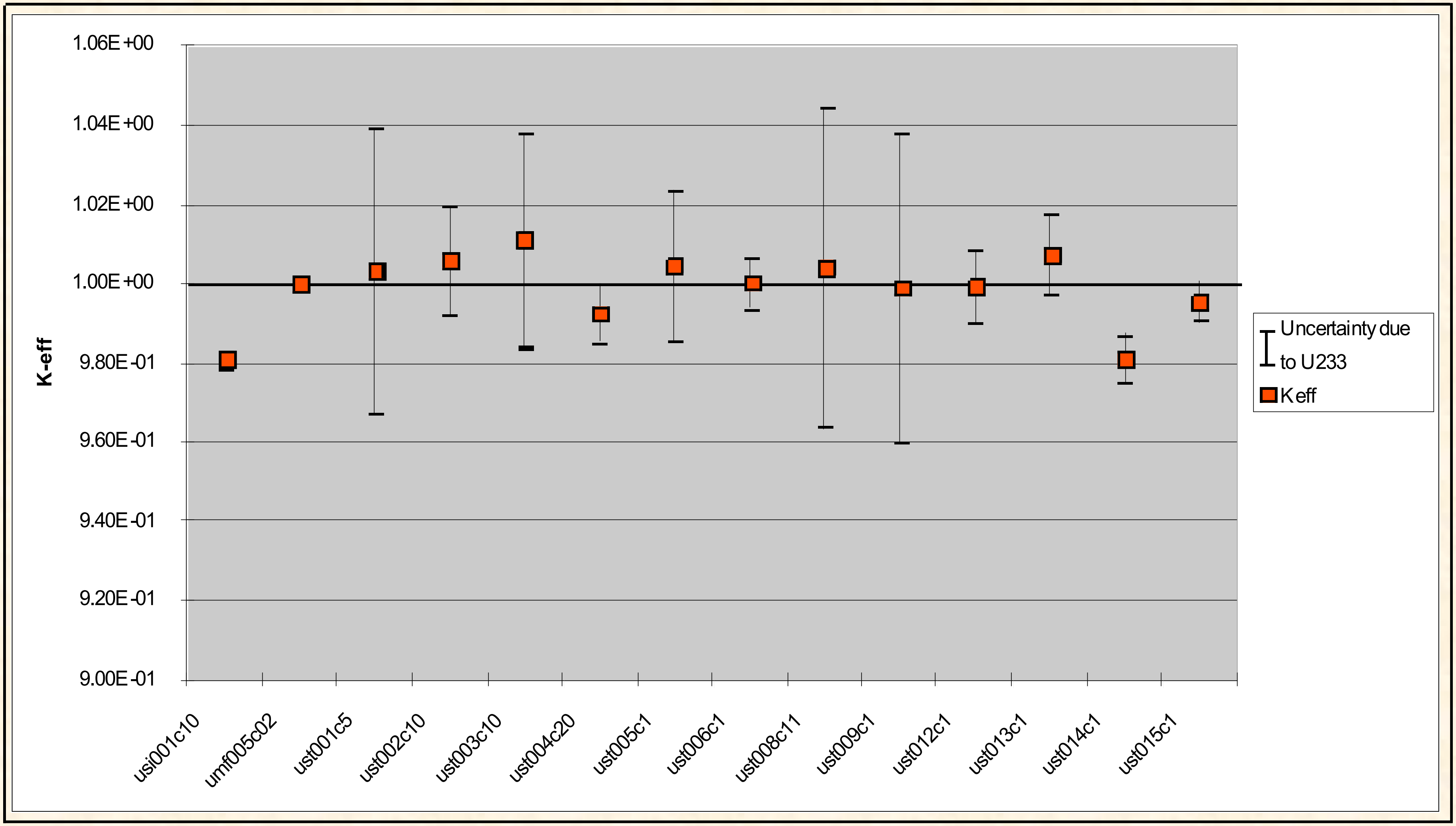


A series of criticality studies were performed at Lawrence Livermore National Laboratory in the late 1950's using aqueous solutions of ^{233}U in the form of UO_2F_2 stabilized with 0.3% by weight of HF.

Sensitivity to the capture and fission cross section for the u233-sol-therm-015 benchmark



Uncertainties Due to ^{233}U Cross Section



Summary

- New evaluated covariance data can be made available by either retroactively generating covariance data or developing a new cross-section evaluation
- Approximate covariance data can be used to fill gaps not covered by current evaluated data
- ORNL has integrated nuclear program in place to address resonance-region data needs
  - Cross-section measurement and evaluation
    - Retroactive covariance evaluation approach can be used to address “short-term” covariance data needs
    - Traditional evaluation approach can be used to rigorously address more “long-term” data needs
  - Cross-section processing methods to prepare libraries from latest ENDF/B covariance formats
  - Radiation transport methods that include 1-D and 3-D sensitivity/uncertainty analysis tools—provides capability to investigate data needs and design experiments
- NNSA/NCSP (NA-11) providing support for development of covariance data for “high-priority” nuclides needed for criticality safety applications in DOE complex
- NCSP cannot single-handedly address data needs for all materials
  - Some overlap with AFCI/GEN-IV resonance-region data needs
  - Need to identify where ORNL can help fill the low-energy data gap for AFCI/GEN-IV

Results from u233-sol-therm-015 benchmark (case 1)

Forward Calculation k_{eff} : 0.99470367

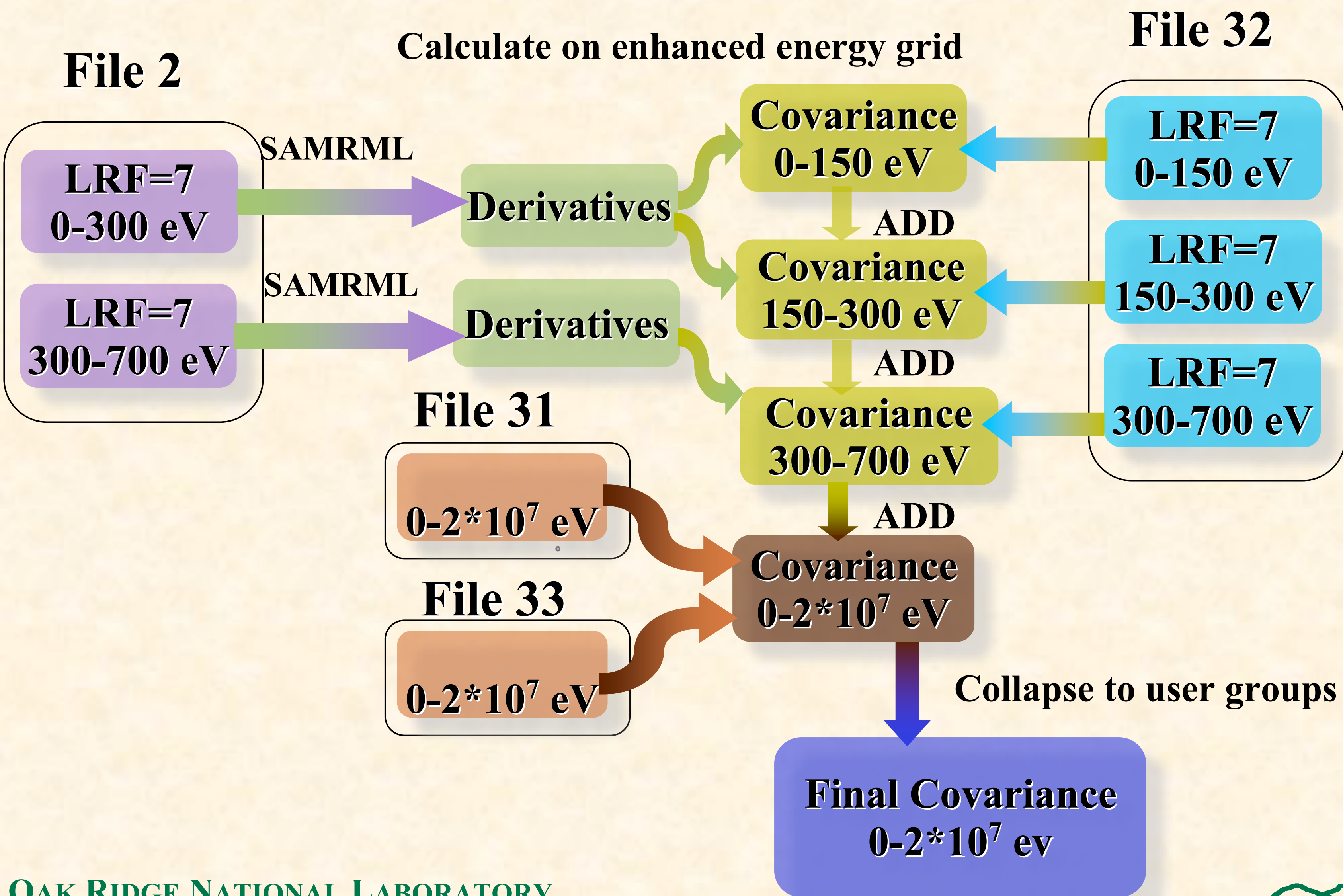
Adjoint Calculation k_{eff} : 0.99451532

Uncertainty in k_{eff} due to ^{233}U cross-section error: 0.5112%

^{233}U Contributions $*10^4$ by reaction pairs to relative covariance of k_{eff}

	fission	n, gamma	elastic
fission	3.9622E-01	-1.0552E-01	-2.4250E-06
n, gamma	-1.0552E-01	7.9620E-02	9.8695E-07
elastic	-2.4250E-06	9.8695E-07	3.0737E-08

Example PUFF-IV Processing Flow Diagram



PUFF calculation of file 32 covariances

Cross section from file 2: $\acute{o}_m(E) = \acute{o}_m(E, P_j)$

The covariance for the parameters is: $Cov(P_i, P_j) = \langle \ddot{a}P_i ; \ddot{a}P_j \rangle$

The propagated covariance for cross section:

$$\langle \ddot{a}\acute{o}_m(E_i)\ddot{a}\acute{o}_l(E_j)\rangle = \left\langle \sum \frac{\partial \acute{o}_m(E_i)}{\partial P_k}\ddot{a}P_k \sum \frac{\partial \acute{o}_l(E_j)}{\partial P_n}\ddot{a}P_n \right\rangle$$

$$= \sum \frac{\partial \acute{o}_m(E_i)}{\partial P_k}\langle \ddot{a}P_k \ddot{a}P_n \rangle \frac{\partial \acute{o}_l(E_j)}{\partial P_n}$$

Group averaged covariance:

$$\langle \ddot{a}x_I^m \ddot{a}x_J^l \rangle = \frac{1}{\ddot{O}_I \ddot{O}_J}\int \ddot{O}(E_i)\langle \ddot{a}\acute{o}_m(E_i)\ddot{a}\acute{o}_l(E_j)\rangle \ddot{O}(E_j)\, dE_i\, dE_j$$

Separating the integral and substituting a sum for the integral

$$\langle \mathrm{\ddot{a}x}_\mathrm{I}^\mathrm{m} \mathrm{\ddot{a}x}_\mathrm{J}^\mathrm{l} \rangle = \sum \mathrm{D}_\mathrm{Ik}^\mathrm{m} \langle \mathrm{\ddot{a}P_k \ddot{a}P_n} \rangle \mathrm{D}_\mathrm{Jn}^\mathrm{l}$$

with $\ddot{O}_I = \sum \ddot{O}(E_i)\ddot{A}E_i$ and $D_{Ik}^m = \frac{1}{\ddot{O}_I}\sum \ddot{O}(E_i)\frac{\partial \acute{o}_m(E_i)}{\partial P_k}\ddot{A}E_i$